

U.S. ARMY CHEMICAL AND BIOLOGICAL DEFENSE COMMAND

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DEVELOPMENT OF A MULTI-CHANNEL INTEGRATION ROUTINE IN LABVIEW®

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GUILD ASSOCIATES, INC. Baltimore, MD 21236

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PREFACE

The work described in this report was authorized under Contract No. DAAA15-93-C-0070. This work was started June 1994 and completed December 1994.

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DEVELOPMENT OF A MULTI-CHANNEL INTEGRATION ROUTINE IN LABVIEW®

1. INTRODUCTION

We developed a general purpose, software-implemented, multi-channel integrator under LabVIEW® version 3.0.1 on a Macintosh Quadra 950 that replaces external hardware based integrators. Specifically, the HP-5880A and the HP-3396 Series II Integrators used for chromatographic analyses can be replaced by any computer with a data acquisition card. The integration routine runs concurrently with other data acquisition and control (DAQ&C) applications under LabVIEW, thus eliminating the need for additional hardware.

The integrator takes any analog output signal from any instrument thus alleviating the necessity of purchasing and supporting integration hardware from multiple vendors. Specific communications drivers do not need to be written for the wide variety of hardware based integrators to interface them with the DAQ&C system. Post analysis of the data is also simplified. Unlike paper-based integrators, further processing of the acquired data does not require re-typing the data into a computer. Not only does this save time, but accuracy is improved. Furthermore, the raw signals may be stored in files for later re-integration or fed to other data analysis programs for specialized treatment.

The software based multi-channel integrator monitors and analyzes more than one channel simultaneously. In situations where simultaneous sampling and/or multiple detectors are required, this software replaces several paper-based integrators such as the HP-5880A and/or HP-3396 Series II Integrators. The HP-3396 Series II integrates up to two channels, but displays only one trace during the acquisition. Integration of four signals simultaneously requires a minimum of two integrators. (Concurrent display and analysis of four channels would require four HP integrators.) Use of the software based integrator eliminates hardware expense associated with the purchase of separate integrators for each channel and space and supervision requirements which are at a premium in a busy lab environment.

Use of this code in existing and future systems will also overcome one of the major limitations of paper-based integration systems: the paper out condition. Paper out conditions cause loss of data in some instances and may interfere with other DAQ&C functions. Further, separate communications routines are not necessary for each model of integrator in use which will minimize system development costs.

The integration program is fully software implemented in LabVIEW, and is easily integrated into any LabVIEW program requiring integration analyses. The code avoids system

specific commands within LabVIEW that would complicate transfer to other platforms. In its current state, the integrator will run on Macs, DOS based machines, and Suns with little more than a re-compilation of the code.

THEORY OF OPERATION

2.1 <u>Data Acquisition</u>.

The system analyzes the raw 0-1 V analog input signal from a gas chromatograph or other instrument and detects the beginning, apex, and end points of the peak. The input resolution is approximately 300 μ V because the MIO board is currently configured for a 10 V bipolar range. Higher resolution is possible by re-configuring the I/O hardware to a smaller, unipolar range of 0-5V. Although this increases the sensitivity of the integration system to detect changes as small as 20 μ V, it can interfere with the detection of higher level signals necessary for other process control features of a given system.

The system samples the input channel at 1000 Hz and averages each set of 50 points to return an effective input to the integrator of 20 Hz. Over sampling is necessary to reduce the effects of noise in the signal. In excessively noisy environments, faster scan rates can be employed, but the integrator always normalizes the input to an effective rate of 20 Hz by averaging more points. The front panel of the VI displays all incoming data on the screen as it is acquired.

2.2 <u>Peak Detection</u>.

Peaks are detected in near real-time as the data is acquired. Both the first and second derivatives are monitored continuously for changes that indicate the beginning, apex, and termination of a peak. The beginning of a peak is detected by monitoring the second derivative of the data for any condition where it remains above the noise level of the signal for a set period of time only when there have been no recent negatively sloped sign changes in the first derivative. This is accomplished by setting a threshold (or noise) limit below which all changes in the signal are ignored and recording the first point above the threshold. The length of time that the second derivative has to be above the threshold limit to be considered a valid event is determined by the peak width. (The peak width parameter is not actually the width of the peak. This parameter is used to measure the <u>duration</u> of the second derivative above the threshold in acquired data points. Data points are currently acquired every 0.05s.)

Once a start event (beginning) of a peak is detected, the program monitors the first derivative for a negatively sloped sign change which is taken as the apex of the peak. The end of a peak is detected similarly to the beginning but it is recorded as the point where either the first

or second derivative is within the threshold limit. All of the events are recorded as indices and labeled with the program's best estimate of the type of event.

2.3 Controlling Integration.

Each channel has parameters that can be set to control peak detection, display, integration, and report generation. The threshold and peak width values completely specify the detection of peaks during the acquisition. The threshold value determines the magnitude of change in either the first or second derivative that is considered to mark a valid event during the integration. (Typical values encountered so far are on the order of 1.0E-6 V.) The peak width parameter is a little misleading: it defines the duration of a threshold event necessary to be considered a valid plot feature, not the width of a peak. Typically, this value is set to three so that the threshold condition must be met for three consecutive points (0.15 sec) in order for the program to consider it a valid plot feature and not transient noise.

The attenuation parameter controls the display of data in the screen. This value currently has no effect on the integration or peak detection, but only scales the data to the graph. The data is scaled by a factor of 2^n so that wide ranges of peak heights can be displayed on the same graph. The functionality of this parameter may be changed later to a more traditional role to aid in the detection of peaks.

The baseline type is the only parameter that affects the integration of the detected peaks since it determines how the baseline is generated for a given plot. The following options are supported: 1) set at beginning, 2) horizontal to lowest point, 3) valley to valley, and 4) least slope line. The set at beginning option and the horizontal to lowest point options are useful for stable baselines. Both generate a baseline that is horizontal and differ only by the level selected for the baseline. Set at beginning creates a horizontal baseline at a level based on the average of the first 5 seconds of data acquired for a given plot while horizontal to lowest point finds the lowest point recorded in the plot and draws a horizontal line through it.

When the baseline is unstable, drifts, or changes throughout the course of an experiment, the remaining options permit reliable integration of peak areas. For a slowly drifting baseline, the least slope line option sets the baseline as the least slope line that goes through the lowest recorded point and another valley point. Valley to valley sets the baseline to run from the start point of each peak to the endpoint of each peak.

Area reject is the only option available to control the report generation from the integrator and acts as a filter which ignores any peak with an area below the set level. Any peak with an area less that the area reject is excluded from the report and all subsequent calculations such as area %.

2.4 Report Generation.

The integrator returns a report of all peaks encountered in the integration and includes the following values for each channel: retention time (RT) in minutes, peak area in counts ($1/8 \mu V$ -sec), peak type, peak width at half height, and percentage of the total area reported that the peak represents. The retention time is determined by fitting a 2nd order equation to the 5 points immediately surrounding the detection of a sign change in the 1st derivative. Two leading and two trailing points are used along with the point of sign change for this analysis. Using this method increases the repeatability of the RT and helps to smooth out any noise and/or error induced by the sampling method.

The area is calculated by numerical integration of the recorded data based on the beginning and end indices detected during the acquisition. The integration uses the Bode Rule to calculate the area under the curve. Since the Bode rule is a fifth order approximation, there is always the possibility that there will not be an integral number of partial sums to complete the calculation. In these cases, the Bode rule is used to the extent possible and the final sums are calculated using the appropriate lower order rule. The progression of lower order rules is as follows: Trapezoidal Rule (2nd order), Simpson's Rule (3rd order), Simpson's 3/8 Rule (4th order).

Once the areas have been calculated, the baseline area is subtracted and the final value is reported in counts. The definition of a count is $1/8 \mu V$ -second. This definition has been chosen to maintain conformity with the HP-3396 Series II integrator as a means for direct comparison of the output data.

Each peak is labeled with a two letter code describing the conditions prevalent at the beginning and end of the peak called the peak type. The first letter describes the start conditions and the second describes the end conditions. Peak type is currently limited to recording baseline, valley, and penetration of baseline events. Baseline (B) marks those events occurring at the baseline within the tolerance set by the threshold while valley (V) marks any event occurring above the baseline. Penetration (P) marks events that occur below the baseline. No provision has been made to detect solvent or other types of peaks.

Finally, the peak width and the percent of the total area reported are calculated for each peak. The peak width is reported in minutes and is the actual width of the peak at half-height. Half height is defined as one half the distance between the apex of the peak and the baseline at that point. (Note that the peak width parameter in the report and the peak width setting for integration are not the same.) The area % is the percentage of the total area reported that is due to a given peak. Peaks with areas below the area reject are not reported and are not included in the area % calculation.

2.5 Other Options.

The integration routine runs either manually or programmatically. In either case, integration and acquisition automatically stop at the end of the value set in run time and the report is generated. In manual mode, start and stop buttons appear in the lower right hand corner of the panel. The program automatically determines the proper mode of operation based on the presence or absence of occurrence parameters.

The program offers complete programmatic control via occurrences when used as a sub VI in another program. The following hooks are available for control: ready, start, external event, and stop. When used as a sub-vi, all trigger values must be set even if a specific trigger is not used. The ready trigger is an occurrence sent and read by the calling program. The calling program must wait for the ready trigger to be sent before sending a start trigger to the integrator. The ready trigger was added to the program to overcome delays caused by the analog input configuration routine. Configuration takes a small amount of time and can cause a visual delay between the sending of a start signal and acquisition of data by the program. Therefore, the integrator sets up the acquisition and then sets the ready occurrence.

Once the integrator is ready, acquisition begins immediately upon receipt of the start trigger. The interaction of ready and start allow precise control of start of the acquisition for time sensitive applications. After receiving the start trigger, the integrator acquires data for the length of time set in the run time parameter and returns a report.

Because the integrator places a significant load on system resources, external timing cannot be relied upon to perform functions such as sample injection at specific times after the start of the acquisition. The external event trigger overcomes this obstacle by setting an occurrence that allows precise timing of an event from within the integration routine. Currently, the external event occurs at two seconds into the acquisition. The timing of this trigger is not user definable.

Although the stop trigger is not currently implemented, it will be used to stop the acquisition at any time before the run time has expired. Upon receiving this trigger, integrator will immediately stop any acquisition in progress and return the current data.

Manual operation disables all triggers but will not clear occurrence values left over from previous programmatic operation. Therefore, manual operation may not work properly immediately after programmatic control unless all triggers are cleared. Triggers can be cleared by re-initializing all values to default before running. Once cleared, triggers cannot be set manually from the front panel of the integrator.

2.6 <u>Error Handling</u>.

When errors are encountered in the acquisition the integrator halts and no data is processed. All data for the current acquisition is assumed to be suspect under these conditions and is discarded without notice. Manually starting or stopping by trigger (when implemented) should provide normal post processing for all data collected to that point.

3. APPARATUS

A typical LabVIEW data acquisition and control system consists of 1) a computer and 2) a multi-function I/O (MIO) board. The integrator requires one differential analog input for each channel. In order to increase the number of I/O operations either another MIO board is added or an SCXI chassis is used to multiplex more signals into a single MIO board. The SCXI option provides the most flexibility and thus that is system used for the following tests.

Both hardware and software were required to test the system. Since none of the GC's (HP-5880) available at our site were equipped with an analog output boards, a data generation program was written that was capable of handling multiple simultaneous analog output signals. (Note, most newer GC's have an analog output option built in to the system and require no additional hardware.)

3.1 Hardware.

The test system consisted of a Macintosh Quadra 950 running system 7.1. Three National Instruments DAQ cards were installed in the computer for the purpose of the test. The installed boards were 1) High Resolution Multifunction I/O board (NB-MIO-16XL), 2) Block Mode DMA and GPIB Interface board (NB-DMA-2800) and 3) Six Channel Analog Output board (NB-AO-6). The cards resided in slots 2-4 of the host computer respectively and were interconnected via the National Instruments Real Time System Integration Bus (RTSI).

The current system uses a National Instruments NB-MIO-16-X I/O card capable of 55,000 samples per second. Ignoring the problems associated with the processor speed inside the Mac itself, a maximum of 55 channels could be processed at once at the current 1000 Hz acquisition rate. Realistically, the total number of channels will probably be around 4 when other control options such as process control and other DAQ channels are added to the processor's load.

The MIO board generated and acquired the test signal. Although the data generation and acquisition occurred completely on the MIO board, the DMA and the AO board were required to generate the signal and re-acquire it completely and reliably on the MIO board.

The DMA board provided increased speed by allowing direct memory access and the analog output board is required by certain subroutines within LabVIEW to generate wave forms.

The MIO board was connected to the Multiplexer module in an SCXI-1001 12-slot signal conditioning chassis via an SCXI-1345 shielded 10m cable (NI# 776574-450) The chassis contained 6 modules: a 32 Channel Multiplexer Amplifier (SCXI-1100), a Feed Through Panel (SCXI-1180), a 16-Channel SPDT Relay Module (SCXI-1160), an 8-Channel Isolation Amplifier (SCXI-1120), and two 6-Channel Isolated Digital to Analog Converters (SCXI-1124). The modules resided in slots 1 - 6 respectively. Only the multiplexer and the feed through were used in this experiment. The other modules in the chassis are listed for completeness, but should have had no effect on the experiment.

Analog input connections were made to the Multiplexer via an SCXI-1300 terminal block with wires connected to channel 6. The negative leg of the input signal was referenced to chassis ground within the SCXI-1300 terminal block. The analog output signal was wired to the multiplexer and the HP-3396 via an SCXI-1302 terminal block connected to the feed through panel. Analog output signals were wired to terminals 20 and 23 which correspond to analog output channel 0 from the MIO board.

3.2 <u>Software</u>.

A multi-channel analog data generator was written to test the multi-channel integrator. The data generator writes a user definable waveform of arbitrary length representing a chromatograph to analog output channel. The program can output as many waveforms as there are analog output channels available. In the present case, only one, 1798 point waveform was used. The data output rate is continuously variable within the bounds of the hardware capabilities and can be set from the front panel.

4. PROCEDURE

The software integrator was tested against the HP-3396 with a simulated chromatogram output at two different rates from the multi-channel data generator. The data output consisted of a triplet of three peaks occurring closely together followed by two overlapping peaks. The two rates used were 20 and 100 Hz. Different rates were used to simulate various elution times. The 100 Hz generation ran for 0.30 minutes (approximately 18 seconds) and was used to test the ability of the integrator to track peaks that appear in rapid succession. The 20 Hz generation provided a more reasonably paced elution scenario during a typical run time of about 1.5 minutes

Slower generation rates were not used because the integration routine would have seen plateaus due to the digital nature of the signal and the limited resolution of the DAC. The signal would not have reasonably simulated an analog signal which would severely compromise the validity of the test. The 20 Hz signal was used as the low limit since that is the same rate at which the integrators process the data. Step changes on the order of 20 Hz should therefore be interpreted as occurring continuously.

For each test, the signal generator was started, and then an integrator was started as soon as practicable. The lag time between the start of data generation and acquisition by the HP-3396 was typically less than that for the software based integration routine since the HP-3396 didn't have to wait for the system to switch between programs. In the worst case, the difference between the start of generation and acquisition was less that 5 seconds.

Under both generation rates, the integration routine was re-tested with the addition of a capacitor installed across the input leads into the multiplexer which provided simple hardware filtering using and RC circuit. (The resistance value was approximately 820 Ω and the capacitor was approximately 2 μ F which provided approximately 40 - 60 Hz filtering.) The exact value of the capacitor was not measured, and the value of the resistance is inherent in the SCXI-1100 module itself. The resistance value of 820 Ω is not directly measurable and is provided by National instruments as a guide and may vary slightly from module to module.

5. EXPERIMENTATION RESULTS

Table 1 compares the report results obtained from the HP-3396 (Figure 1) and the integration routine (Figure 2) for the 1.5 minute run for an unfiltered input signal. Due to the noise inherent in the signal, the integration routine detected a second peak at 1.179 minutes. Based on the data in the table, it is very likely that this peak should have been integrated as part of the peak at 1.155 minutes. In fact, addition of the areas for 1.155 and 1.179 yields 663576 counts which compares very favorably with HP results of 666290 counts for the 1.168 minute peak. Treating the area %'s similarly yields 9.81422 % which also compares favorably with the HP value of 9.45948%.

The effects of the addition of a filter to the input signal to the integration routine can be seen by comparing Figures 2 and 3. In Figure 2, the chromatogram appears noisy, but continuous. The addition of hardware filtering cleans up the signal appreciably, and the stepwise nature of the input signal is quite apparent in Figure 3. More importantly though is the appearance of the baseline. What appears as a noisy baseline in Figure 2, is reduced to an extremely clean and flat baseline in Figure 3. (Similar results apply to Figures 5 and 6 but are less apparent.)

With signal filtering, it appears as though the LabVIEW did not register the valley of the overlapping peaks properly around 1.3 minutes but appears to have integrated it as a single peak. Addition of the areas reported for retention times 1.168 and 1.244 minutes by the HP-3396 yields 1662328 counts. The integration routine found 1504778 counts for the combined peak at 1.300. This area is still a little low and the peak detected at 1.324 minutes with 79113 area counts is probably part of this also.

The integration routine appears to have some trouble detecting valleys properly. It is probable that some modification of the threshold and peak width inputs will increase the sensitivity. Slight variations in the retention time are partially or wholly attributable to the manual start operation. In both cases the software integrator did not detect the small peak at approximately 0.619 minutes. It is impossible to tell whether the peak was missed completely or was rejected due to the relatively large area reject value of 30, 000 counts. The HP area reject was set at 0.

Tables 3 and 4 compare the results for the 0.30 minutes unfiltered and filtered inputs respectively. In these tests, the data generation rate may have been too fast for both HP-3396 and the integration routine. Both integrators reported only three out of the five peaks in the data set. The first triplet of peaks should occur at approximately 0.08, 0.100, and 0.140 minutes respectively. Both integrators seem to have missed the first peak, and captured the other two. Although the integration routine returned somewhat lower values than did the HP-3396, the results are encouraging.

The overlapping double peak should have occurred around 0.210 and 0.240 minutes. It appears as though the HP integrator captured the double peak as a single peak at 0.245 minutes since type is listed as PB (Penetration/Baseline). In contrast, the integration routine seems to have found only the first peak since type is PV (Penetration/Valley). The second peak may have been detected and been rejected due to the area reject of 30, 000 counts.

The results from the integration of filtered input are quite similar to that obtained for unfiltered input where the overlapping peaks at 0.21 - 0.240 min. are concerned. As in the unfiltered example, it appears as though the HP integrator captured the double peak as one since the type is PB and the soft integrator only found the first peak since type is PV. The most significant difference occurred in the detection of the peaks of the first triplet. In this case, the soft integrator seems to have detected the first peak of the triplet and missed the second which is the opposite behavior observed for the HP-3396. Both integrators reliably detected the third peak with similar areas.

The accuracy of the digital to analog converter (DAC) limits the resolution of the output. In the test case the DAC had a resolution of 12 bits and was set for an output range of

+/- 10 V. The result can be seen as steps in the actual chromatogram in Figures 3 and 6. This may be another reason for false ends and starts resulting in inconsistent area counts and peak detection between the HP and software based integrators.

6. CONCLUSIONS

An integration routine was developed under LabVIEW version 3.0.1 on a Macintosh Quadra 950 that is capable of continuously monitoring and displaying as many channels as can be physically linked into the data acquisition system. The addition of other acquisition and control functions running on the same processor will have a significant effect on the maximum number of channels that can be integrated reliably.

The system has been tested with simulated input signals and the results compared to those obtained from an HP-3396 Series II integrator. Overall, the results obtained from the integration routine show that peaks can be detected and integrated with results similar to those obtained from a commercial stand-alone unit. The lack of advanced features and difficulty in handling valley points limit the use of the integration routine to extremely simple chromatograms. Further development should increase performance and reliability.

Results obtained from both filtered and unfiltered input imply that some sort of filtering beyond simple oversampling and averaging will be necessary. Improvements in the signal quality may be realized by the addition of a simple RC circuit to the input. Due to the nature of the inherent resistance of the input device (in this case, SCXI-1100), some trial and error may be necessary to find the optimum capacitance for the filter circuit. More sophisticated filtering methods may have to be employed in extremely noisy environments.

There are various improvements that can be made to make the program more versatile and more memory efficient. Future improvements will include: 1) the addition of an event table to allow changes in the previously described parameters during the course of a run, 2) provision for handling and properly recording solvent and associated rider peaks, 3) addition of de-convolution routines for the separation of overlapping peaks, and 4) creation of a calibration table to allow translation of the peak data into absolute units such as concentration or mass.

Further testing should also be conducted to determine the reliability and repeatability of the results obtained from the integration routine. The system should be tested with a true analog signal from a GC or other instrument. Multiple tests should also be conducted in order to compare the consistency of the results between runs.

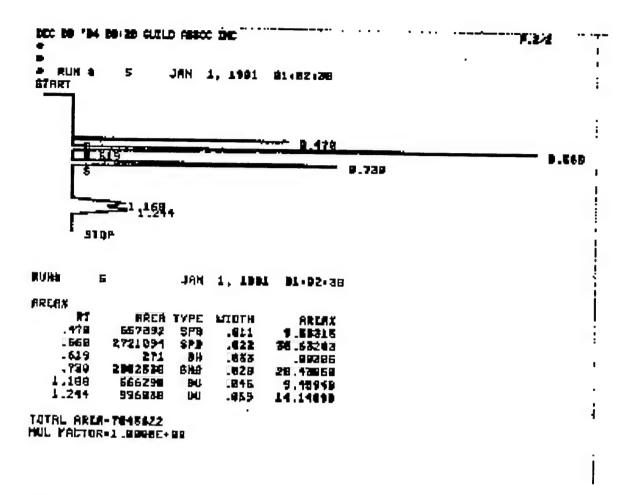


Figure 1. Output from the HP-3396 Series II integrator for the 1.5 minute test. The data consisted of 1799 data points output from the computer at 20 Hz and read as a 0-1V analog input to the integrator.

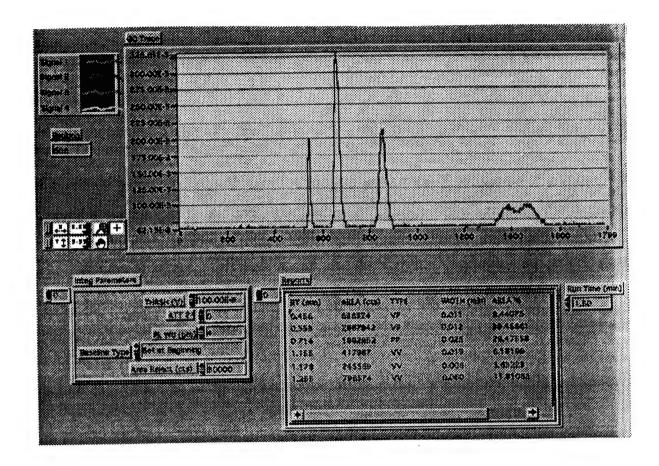


Figure 2. Front panel display of the multi-channel integrator after the unfiltered 1.5 minute test. The data consisted of 1799 data points output from the computer at 20 Hz and read into the integrator at an effective rate of 20 Hz.

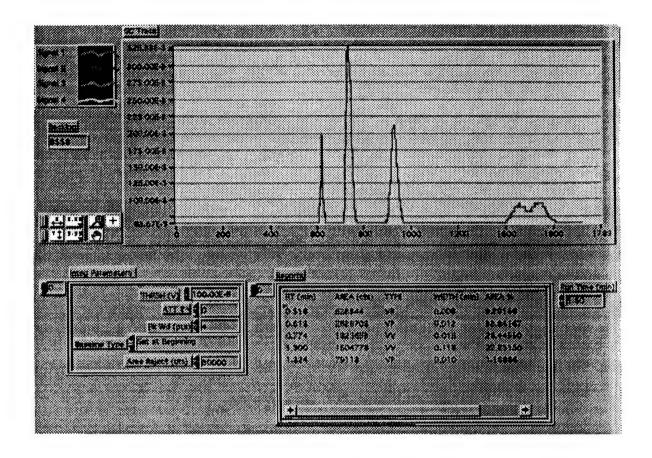


Figure 3. Front panel display of the multi-channel integrator after the filtered 1.5 minute test. The data consisted of 1799 data points output from the computer at 20 Hz and read into the integrator at an effective rate of 20 Hz. hardware filtering was achieved by inserting a 2.2μF capacitor across the input leads to remove noise.

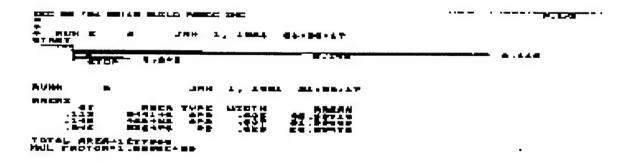


Figure 4. Output from the HP-3396 Series II integrator for the 0.30 minute test. The data consisted of 1799 data points output from the computer at 100 Hz and read as a 0-1V analog input to the integrator.

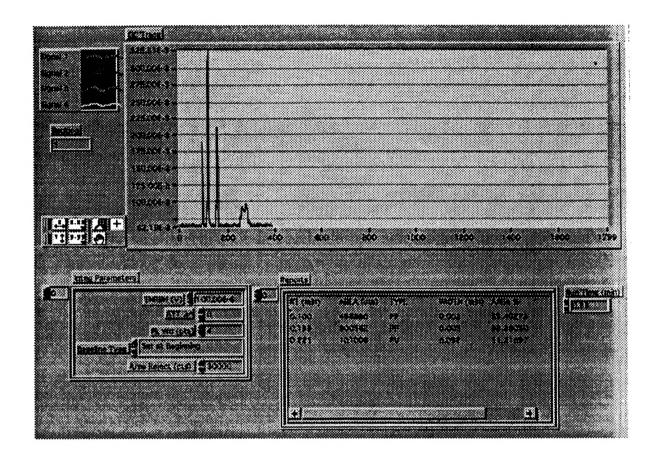


Figure 5. Front panel display of the multi-channel integrator after the unfiltered 0.30 minute test. The data consisted of 1799 data points output from the computer at 100 Hz and read into the integrator at an effective rate of 20 Hz.

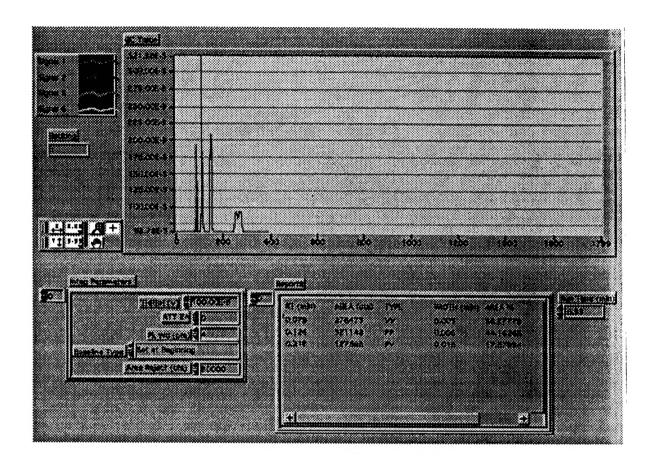


Figure 6. Front panel display of the multi-channel integrator after the filtered 0.30 minute test. The data consisted of 1799 data points output from the computer at 100 Hz and read into the integrator at an effective rate of 20 Hz. hardware filtering was achieved by inserting a 2.2μF capacitor across the input leads to remove noise.

Table 1. Comparison of results from HP-3396 Series II integrator and Guild Integrator for the 1.50 minute run with unfiltered input. The results provided are: retention time in minutes (RT), peak area in counts (AREA), type of peak detected (TYPE), peak width at half height (WIDTH), and percentage of the total area detected (AREA %). The results for the HP3396 are listed under HP and those for the integration routine are listed under LV. N/D means not detected.

| R | Т | AR | EΑ | TY | PE | WIL | TH | ARE | A % |
|-------|-------|---------|---------|-----|-----|-------|-------|----------|----------|
| HP | LV | HP | LV | HP | LV | HP | LV | HP | LV |
| 0.470 | 0.456 | 657392 | 638324 | SPB | VP | 0.011 | 0.011 | 9.33315 | 9.44075 |
| 0.568 | 0.553 | 2721094 | 2667942 | SPB | VP | 0.022 | 0.012 | 38.63203 | 39.45861 |
| 0.619 | | 271 | N/D | ВН | N/D | 0.033 | N/D | 0.00385 | N/D |
| 0.730 | 0.714 | 2002536 | 1992952 | SHB | PP | 0.028 | 0.022 | 28.43050 | 29.47558 |
| 1.168 | 1.155 | 666290 | 417987 | BV | VV | 0.046 | 0.019 | 9.45948 | 6.18199 |
| N/D | 1.179 | N/D | 245589 | N/D | VV | N/D | 0.008 | N/D | 3.63223 |
| 1.244 | 1.255 | 996038 | 798574 | VV | vv | 0.069 | 0.060 | 14.14099 | 11.81083 |

Table 2. Comparison of results from HP-3396 Series II integrator and Guild Integrator for the 1.50 minute run with filtered input. The results provided are: retention time in minutes (RT), peak area in counts (AREA), type of peak detected (TYPE), peak width at half height (WIDTH), and percentage of the total area detected (AREA %). The results for the HP3396 are listed under HP and those for the integration routine are listed under LV. N/D means not detected.

| R | T | AR | EΑ | TY | PE | WII | OTH | ARE | A % |
|-------|-------|---------|---------|-----|-----|-------|-------|----------|----------|
| HP | LV | HP | LV | HP | LV | HP | LV | HP | LV |
| 0.470 | 0.516 | 657392 | 628344 | SPB | VP | 0.011 | 0.008 | 9.33315 | 9.29146 |
| 0.568 | 0.613 | 2721094 | 2626703 | SPB | VP | 0.022 | 0.012 | 38.63203 | 38.84167 |
| 0.619 | N/D | 271 | N/D | ВН | N/D | 0.033 | N/D | 0.00385 | N/D |
| 0.730 | 0.774 | 2002536 | 1923653 | SHB | vv | 0.028 | 0.018 | 28.43050 | 28.44550 |
| 1.168 | 1.300 | 666290 | 1504778 | BV | VV | 0.046 | 0.118 | 9.45948 | 22.25150 |
| 1.244 | N/D | 996038 | N/D | VV | N/D | 0.069 | N/D | 14.14099 | N/D |
| N/D | 1.324 | N/D | 79113 | N/D | VP | N/D | 0.010 | N/D | 1.16986 |

Table 3. Comparison of results from HP-3396 Series II integrator and Guild Integrator for the 0.30 minute run with unfiltered input. The results provided are: retention time in minutes (RT), peak area in counts (AREA), type of peak detected (TYPE), peak width at half height (WIDTH), and percentage of the total area detected (AREA %). The results for the HP3396 are listed under HP and those for the integration routine are listed under LV. N/D means not detected.

| R | Т | ARE | A | TY | PE | WIDTH | | ARE | A % |
|-------|-------|--------|--------|-----|----|-------|-------|----------|----------|
| HP | LV | HP | LV | HP | LV | HP | LV | HP | LV |
| 0.112 | 0.100 | 544145 | 498890 | SPB | PP | 0.005 | 0.002 | 42.60918 | 55.40273 |
| 0.145 | 0.133 | 400436 | 300582 | SPB | PP | 0.007 | 0.005 | 31.35608 | 33.38030 |
| 0.245 | 0.221 | 332479 | 101006 | PB | PV | 0.023 | 0.032 | 26.03473 | 11.21697 |

Table 4. Comparison of results from HP-3396 Series II integrator and Guild Integrator for the 0.30 minute run with filtered input. The results provided are: retention time in minutes (RT), peak area in counts (AREA), type of peak detected (TYPE), peak width at half height (WIDTH), and percentage of the total area detected (AREA %). The results for the HP3396 are listed under HP and those for the integration routine are listed under LV. N/D means not detected.

| R | Т | ARE | CA | TY | PE | WII | TH | AREA % | |
|-------|-------|--------|--------|-----|-----|-------|-------|----------|----------|
| HP | LV | HP | LV | HP | LV | HP | LV | HP | LV |
| N/D | 0.079 | N/D | 278475 | N/D | VV | N/D | 0.005 | N/D | 38.27778 |
| 0.112 | N/D | 544145 | N/D | SPB | N/D | 0.005 | N/D | 42.60918 | N/D |
| 0.145 | 0.124 | 400436 | 321143 | SPB | PP | 0.007 | 0.005 | 31.35608 | 44.14268 |
| 0.245 | 0.212 | 332479 | 127893 | PB | PV | 0.023 | 0.013 | 26.03473 | 17.57954 |